

Proposal – Annex 22

**FUNDAMENTAL AND APPLIED HYDROGEN STORAGE
MATERIALS DEVELOPMENT**

Prepared for

**Executive Committee
IEA Hydrogen Implementing Agreement**

by

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1. Background – The Need for Hydrogen Storage

During the last decade there has been a significantly increased focus on hydrogen as the future energy carrier. The main reason is that a hydrogen economy may be an answer to the two major challenges facing the future global economy: climate changes and the security of energy supplies. While many individual scientists and national departments of energy have considered hydrogen fuel a worthwhile goal since the 1971 “energy crisis”, we are now seeing strong interest in many countries with public strategic plans and significant funding efforts (e. g. USA, Japan, Canada, the European Commission) related to hydrogen. In addition the industrial sector, in particular oil companies and automobile manufacturers, are showing increasingly strong interest. The need for new and sustainable energy technologies is particularly urgent in the transport sector where energy demands keep growing and because of the significant global and local pollution. Hydrogen is expected to play a key role in this development. The major components in the expected Hydrogen Economy involve production, storage and final use of hydrogen, e.g. in fuel cells, all of these facing considerable technological challenges.

Hydrogen storage is a crucial step for providing a ready supply of hydrogen fuel to an end use, such as a car. Without effective storage systems, a hydrogen economy will be difficult to achieve. Hydrogen storage remains an undisputed problem for hydrogen-fueled vehicles, and is considered by many to be the most technologically challenging aspect of achieving a hydrogen-based economy. It is also clear that compressed or liquid hydrogen will never meet the long-term goals for hydrogen storage in vehicles. However, in spite of the significant achievements related to hydrogen storage in solid materials during the last years (as discussed below), further progress is still needed to fulfill the international goals, e.g. with respect to gravimetric and volumetric capacities, temperature and pressure for hydrogen release etc. Such research efforts will require new materials and solutions, and not simple, incremental improvements in current technologies.

The annex 17 has grown into the largest international co-operative effort on hydrogen storage ever established. In view of the progress with solid-state H₂-storage under IEA Annex 12 and 17, as well as other non-IEA programs, it seems prudent that further R&D work in this area should be supported in the form of a new IEA H₂ Annex. It is suggested that this new Annex shall cover both fundamental and applied hydrogen storage materials development. This will include development of metal hydrides (both reversible and regenerated chemical hydrides), nanoporous materials and liquid storage media in addition to system and safety aspects. The work will both be experimental and theoretical (modeling).

2. Background – The Lessons of Annex 17

Major activities in Annex 17 “Solid and liquid state hydrogen storage materials” have been on reversible hydrogen storage materials, and in particular complex hydrides and carbon-based materials. In addition, projects on non-conventional interstitial hydrides, regenerative solids (chemical hydrides), tank design (engineering) and safety aspects of the materials have been included in the annex. The annex was also open to rechargeable liquids, but without any running projects. The development of the light-weight reversible hydrides (in particular catalyzed sodium alanate, NaAlH₄) and the promising results for carbon-based compounds (e.g. carbon nanotubes and graphite nanofibers) during the lifetime of Annex 12 were important arguments to decide to form the IEA hydrogen storage Annex 17 in 2001. The first target of Annex 17 was set at 5 wt% H₂ recoverable at <80 °C and 1 atm absolute pressure. Compared to Annex 12 the only change was a somewhat lowered temperature (100 °C in annex 12). The second target for Annex 17 was

to develop the fundamental and engineering understanding of hydrogen storage. At the beginning the task included six countries and 18 official experts for a total effort of about 15-16 person-years/year (py/y). Now, when annex 17 finishes, the number of experts has increased to 38 from 13 countries with a total effort of 44 py/y. This shows the significant increased international interest. The 36 projects have been grouped into (i) metal hydrides; (ii) carbon and (iii) hydrides plus carbon. The number of publications, presentations and patents during the 5 years of task 17 will probably exceed 800. This clearly shows the impact of the Experts in Annex 17 on the development in this field. The participation in Task 17 has significantly contributed to the development of international collaboration among the experts and their research groups.

During the 5 years of Annex 17 the new promising compounds like new alanates, amides/imides systems, borohydrides and different metastable Mg-based materials have been developed in parallel with the development and improved understanding of the effect of catalysts in particular in the alanates. Carbon-based compounds were very promising when Annex 17 started based on several reports of high H-storage capacities, but the data showed poor reproducibility. The problems with reproducibility have been addressed, and a much better basis for evaluation of nanoporous materials has been obtained. The Task 17 targets have not been fully met, but several possible new materials have been developed in Annex 17. The successes of Task 17 clearly show the potential for preparation of new and further significant improvement of hydrides and nanoporous materials. Therefore, continued R&D on hydrides and nanoporous materials are herein proposed.

Sessions related to the safety of the hydrogen storage materials have been held at the workshops in the latter years of the Annex 17. It is important to exchange information about safety aspects of the materials, and materials safety is herein also suggested for inclusion in this proposed new Annex.

Annex 17 included projects related to development of alanate tanks and physical properties of the tanks itself. Such projects will be welcomed for the new proposed Annex.

3. Annex Targets

The Task shall have the following Targets:

- A. Develop a reversible or regenerative hydrogen storage medium fulfilling international targets for hydrogen storage.
- B. Develop the fundamental and engineering understanding of hydrogen storage by various hydrogen storage media that have the capability of meeting Target A.

Annex 12 and 17 had quantitative Targets for hydrogen storage capacity (5 wt%) and temperature for hydrogen release (80 °C in Annex 17). During the years several countries have defined targets for hydrogen storage (e.g. US DOE, Japan and the European Commission). These Targets include a number of parameters important for practical hydrogen storage systems. The Target A for the new Annex is proposed not to be quantitative but instead refer to such national Targets. This gives more flexibility and will also include other relevant parameters than the conventional weight percentage and hydrogen release temperatures.

Target B is more general and has been included to recognize the fact that fundamental understanding of the scientific H-storage mechanisms is limiting in new groups of hydrogen storage media (one example is the role of catalyst in NaAlH₄ that is still not understood). Similarly on the other side of the spectrum, engineering application of these new “exotic”

materials is not always obvious. Both scientific and engineering modeling will be considered in this new Annex, as well as engineering support work necessary for applications.

4. Annex Project Structure

Task 22 will be built on several projects with international collaborations strongly encouraged. Each proposed Project will be based on a short (1-2 pages) Project Plan which will be submitted to the participating ExCo members for formal approval at regular ExCo meetings, starting with the meeting in Autumn 2006 (see also Section 5 for more detail). Each project can include several Experts, but with one Project Leaders who will make the primary judgment as to whether the effort is appropriate for IEA HIA There may be areas that have a large degree of external commercial or quasicommercial interest and are not appropriate for international, relatively open IEA R&D.

Task 22 is open to a broad spectrum of project types:

- A. Experimental
- B. Engineering
- C. Theoretical
- D. Modeling (scientific or engineering)
- E. Safety aspects of hydrogen storage materials

Task 22 will be open to the following classes of H-storage media (the classification is somewhat changed from Task 17, but the same classes of materials are included):

- A. Reversible metal hydrides, including alanates, borohydrides, amides/imides-systems, magnesium-based compounds, alane and mixture of different classes of compounds etc.
- B. Regenerative hydrogen storage materials (chemical hydrides).
- C. Nanoporous materials including carbon, metal-assisted carbons, metal-organic framework compounds (MOFs), zeolites etc.
- D. Rechargeable organic liquids and solids.

All proposed projects will involve H-storage media that offer at least some theoretical hope of achieving Task Target A or will boldly contribute to new fundamental mechanistic understandings as per Task Target B. The above lists should not be considered all-inclusive. The idea of new Annex 22 will be to look at various innovative, “high risk” ideas that have some hope of opening new hydrogen storage areas. At the same time, it will provide the opportunity for engineering development of recently identified H-storage media. Safety aspects will also be an important part of the Annex.

5. Proposed Participation – Countries, Experts, Charter Projects and National Participation Letters

The Task Definition Phase has been completed via preliminary e-mail communications and a Task Planning Workshop in Windermere, UK May 1-4, 2006. The proposed Countries, Organizations, Levels of Effort, Lead Experts and Project Subjects resulting from the Task Planning Workshop are listed in the Annex 22 Participation Table appended to this proposal. 15 countries, 41 organizations and 44 Official Experts are listed with for a total effort of about 56-57 person-years/year (py/y). Universities, National Laboratories and Companies are represented.

Minimum National Participation has been set at 1.0 py/y and all countries meet that minimum, at least at this unapproved proposal stage. All Experts listed in the Table have agreed to participate according to the Implementing Agreement's blanket rules and the specific Task guidelines listed in Part 9 of this proposal, of course subject to available local funding and executed National Participation Letters (NPL) by the respective ExCo members. Prospective Experts will be expected to contact their respective ExCo members to lobby for approval, i.e., inclusion in their country's NPL. The NPL to be used is the standard one used over the years by HIA. It includes a level of commitment and a guarantee of travel funds to the semiannual Experts' Workshops.

Given preliminary approval of this Annex Proposal by the ExCo, all project leaders will be asked to provide an approximately 1-page Project Proposal based on their Windermere presentation plans. These Project Plans will be distributed to the Experts themselves, as well as to the ExCo members for approval by participating Task countries (at a regular ExCo meeting, presumably October 2006). During the first period of the Task (at least the first year), new Experts are welcome when the respective ExCo member has approved participation and their project has been approved by the Official Experts.

In addition to those declared Organizations and Experts listed in the Participation Table, Germany plan to join the IEA HIA very soon (a meeting will be held in Germany these days), and the following German organizations and experts have agreed to participate if it is decided that Germany will be part of IEA HIA and its new ExCo member approves:

- FZK (Official Expert: M. Fichtner): (i) Investigation of the crystal- and electronic structure and the stability of complex borohydrides (1.0 py/y) (proposed together with EMPA, Switzerland); and (ii) Fundamental safety investigations of solid state hydrogen storage materials and systems (1.0 py/y) (part of project with several partners and the USA's Savannah River National Laboratory as project manager).
- GKSS (Official Expert M. Dornheim): Reactive hydride composites (1.0 py/y).
- MPI Stuttgart (Official Expert M. Hirscher): Nanostructures with high specific surface area for hydrogen storage (0.5 py/y).

Professor R. Griessen from Vrije University, Netherlands and professor H. Jonsson, University of Iceland, Iceland have expressed interest and plan to join later.

6. Interaction between IEA HIA and IPHE

Within the hydrogen storage field it is recognized that both IEA HIA and IPHE will be critically important leaders in the international efforts to facilitate the major technical and governmental energy breakthroughs that are needed to create a new hydrogen energy system. The origins and *modi operandi* of the two organizations are different and complementary, but the end objective is the same, the solving of the technical and societal barriers on the road to hydrogen success. The IPHE was created less than three years ago and operates from a base situated at the highest levels of government, both ministerial and energy agencies. The IEA HIA was created 29 years ago and uses as its principal operational bases the various R&D Annexes and the Experts who populate them. Both approaches are needed, and so the two organizations are complementary to a significant extent. The Experts of the proposed Annex 22 have decisively expressed the willingness to collaborate with IPHE on such terms as will be mutually approved by IEA HIA and IPHE. Collaboration can be synergistic and conservational, and can result in less duplication, more real productivity, less travel and redundant meetings and a more rapid solution of the ultimate technical problems. It is hereby proposed to at least invite IPHE scientists and administrators to coming Annex 22 workshops. However, Task 22 fully understands it is a legal instrument of the IEA HIA ExCo and must ultimately defer to its

approval of any such suggestions of a collaborative nature. We support and encourage any legal and procedural discussions the IEA HIA ExCo may have with the IPHE Secretariat toward joint activities, but our duty always lies first with the HIA.

7. Annex Starting Date and Duration

The Task is recommended to start in November 2006, and last for 3 years.

8. Recommended Annex Operating Agent

Professor Bjørn C. Hauback is recommended for the position. He is Deputy Department Head of Physics Department at Institute for Energy Technology (IFE), Kjeller, Norway and also an Adjunct Professor at University of Oslo. Funding for the position is from the RENEGI program in the Research Council of Norway. If approved, he will serve for the three-year duration of Annex 22.

9. Annex Mechanics

- A. Workshops - There shall generally be two Task Workshops per year. The workshops will be independent events with typical duration of 3-4 days. Experts are expected to participate in all Workshops, in person or by proxy giving presentations of their project (or their part of a joint project). Each participating Country will be expected to provide travel funds to its Experts for that purpose, as required of the standard IEA HIA National Participation Letter for it Annexes. To facilitate maximum efforts to solve the hydrogen storage problem, scientists from IPHE countries, can be invited to Task 22 Workshops if so accepted by IEA HIA ExCo.
- B. Annual Reports - The Task shall require 1-2 page annual reports from each Expert. These reports will be published on the web-page for Annex 22 (operated by IFE). In addition, the Experts should submit lists of publications, presentations and patents resulting from the work in the Annex. At the end of the Annex, a 5-6 page report will be required of each project.
- C. Other Reports – All other reports required of an IEA HIA Annex will be promptly and diligently filed by the Operating Agent.
- D. Intellectual Property – Intellectual property developed during this Task will be treated according to MODEL LANGUAGE FOR INTELLECTUAL PROPERTY AND PATENT RIGHTS, Appendix 1C, Handbook of Policies and Procedures for the IEA Hydrogen Program, Third Review Draft, Aug. 1997.

10. Requested of the Executive Committee at the Lyon Meeting

The Task Organizer hereby requests preliminary approval of this Task 22 Proposal, subject to any changes requested by the ExCo. A preliminary poll of national participation is also solicited. Thereafter, between the Spring and Autumn 2006 ExCo meetings, details will be completed: (1) individual project plans; (2) discussions between prospective Experts and their respective ExCo members; (3) National Participation Letters (where possible); (4) etcetera. At the Autumn 2006 ExCo meeting, I shall then ask for final approval of the Task.

Table of Proposed Task 22 Participation

<u>Country</u>	<u>Organization</u>	<u>Pv/y</u>	<u>Official Expert</u>	<u>Title of project</u>
Australia	Curtin U.	3.0	C. Buckley	Light metal complexes for hydrogen storage.
	Griffith U.	2.0	E. Gray	Lithium-based hydrogen storage materials.
Canada	HRI-UQTR	1.0	R. Chahine	H ₂ storage in nanoporous structures.
	HRI-UQTR	1.0	R. Chahine	Fundamental safety investigations of solid state hydrogen storage materials and systems (1).
Denmark	iNANO, Aarhus U.	1.0	T. Jensen	Synthesis and characterisation of light metal hydrides and nanoporous materials.
	Risø National Lab.	1.0	T. Vegge	Crystal structures, stability and hydrogen dynamics in borohydrides and alanates
EC	EC-JRC	1.0	C. Filiou	Gravimetric, volumetric, Temperature-Programmed Desorption. techniques comparison from both hydrogen storage capacity and kinetics point of view.
France	CNRS Grenoble	1.0	D. Fruchart	Nanocrystalline light alloys (Mg, Mg-rich) and complex alloys/nanocatalysts processed by SPD (Severe Plastic Deformation) and high hydrogen pressure.
	CNRS Thiais	1.0	M. Latroche	Hybrid solutions for hydrogen storage.
Italy	CNR-ISC	1.0	M. Zoppi	Microscopic characterization and modelling of hydrogen storage materials (metal hydrides, carbon and nanoporous, clathrates) by Raman spectroscopy and neutron scattering techniques.
	U. of Milan	1.5	A. Albinati	Hydrogen dynamics and lattice interactions in chemical hydrides, carbon nanotubes and metal alloys (2).
	U. of Rome	1.5	R. Cantelli	Hydrogen dynamics and lattice interactions in chemical hydrides, carbon nanotubes and metal alloys (2).

Japan	ETRI AIST	1.0	E. Akiba	Synthesis of novel hydrides with Al-H bonding and characterization of reaction mechanism.
	Hiroshima U.	1.0	Y. Kojima	Hydrogen storage properties of nano-composite materials prepared by mechanical ball milling.
	Kansai U.	1.0	H. Takeshita	Effect of poisoning of LiH in amide – LiH mixture on its hydrogenation properties.
	MERIT	1.0	S. Suda	Sodium borohydride as a hydrogen storage material - Production & regeneration of borohydrides via boron minerals.
	Tohuko U.	1.0	S. Orimo	Light element hydrides for solid-state hydrogen storage – complex and perovskite hydrides.
	UBIQEN/AIST	0.5	N. Kuriyama	International standardized testing protocols for hydrogen storage materials (3).
	UBIQEN/AIST	1.0	N. Kuriyama	Fundamental safety investigations of solid state hydrogen storage materials and systems (1).
Korea	KBSI	1.0	H.-J. Kim	Development and molecular design of nanoporous material for high efficiency hydrogen storage.
	KIGAM	1.0	S.-W. Cho	Development of a high-performance hydrogen storage material using metal hydrides, with design technology for hydrogen storage vessels.
	KIST	1.0	Y.-W. Cho	Synthesis and characterization of complex alloy hydrides.
Lithuania	LEI	1.0	D. Milcius	Development of nanocrystalline metal hydrides using vapour deposition technologies.
Norway	IFE	1.0	B. C. Hauback	Synthesis, structural characterization and stability of complex hydrides.
Spain	ICMAB-CSIC	1.0	J. Iñiguez	Simulations of metal-assisted carbons for hydrogen storage.
Sweden	Stockholm U.	1.0	D. Noréus	Hydrogen storage in metastable lightweight hydrides.
Switzerland	EMPA	1.0	A. Züttel	Investigation of the crystal- and electronic structure and the

				stability of complex borohydrides (4).
UK	ISIS	1.0	B. David	Synthesis, structure and simulation of novel complex hydrides.
	Queen Mary U.	3.0	X. Guo	Theoretical and experimental investigations of hydrogen storage materials.
	U. of Birmingham	1.0	P. Anderson	Hydrogen storage in nanoporous material at room temperature.
	U. of Birmingham	2.0	D. Book	Hydrogen storage in borohydrides and light-metal hydrides.
	U. of Nottingham	2.0	G. Walker	Multicomponent hydride systems.
	U. of Oxford	1.5	P. Edwards	Hydrogen storage in futuristic solids.
	U. of Salford	1.0	I. Morrison	First principles modeling of hydrogen absorption in framework materials.
	U. of Salford	1.0	D. K. Ross	Inelastic neutron scattering studies of hydrogen sorption in solids.
USA	Caltech	0.8	C. Ahn	Enhanced physisorption in Ni modified carbon aerogels.
	Hy-Energy	1.0	K. Gross	International standardized testing protocols for hydrogen storage materials (3).
	GE	2.0	J. C. Zhao	Exploration of $Mg(BH_4)_2$ as a reversible hydrogen storage material.
	ORNL	0.5	N. Gallego	Effect of metal doping on the hydrogen storage capacity of activated carbon fibers.
	Sandia	1.5	D. Dedrick	Fundamental safety investigations of solid state hydrogen storage materials and systems (1).
	SRNL	1.0	D. Anton	Fundamental safety investigations of solid state hydrogen storage materials and systems (1).
	SRNL	1.0	R. Zidan	Development and characterization of novel hydrogen storage materials.
	U. of Hawaii	1.5	C. Jensen	Novel borohydrides for hydrogen storage.
	U. of Nevada	2.0	D. Chandra	Extrinsic effects of impurities on hydrogen metal cycling on Li based hydrides and in-situ diffraction studies on hydriding/dehydriding Li_3N .
	US DOE	0.3	G. Sandrock	IEA/DOE/SNL Hydride Databases.
UTRC	1.5	D. Mosher	Development and application of new high capacity hydrogen	

UTRC	0.5	D. Mosher	storage materials. Fundamental safety investigations of solid state hydrogen storage materials and systems (1).
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Total **55.6 py/y**

- (1) The proposed project “Fundamental safety investigations of solid state hydrogen storage materials and systems” is joint project between SRNL, USA (D. Anton as the project leader), HRI-UQTR, Canada (R. Chahine), UBIQEN/AIST, Japan (N. Kuriyama), Sandia, USA (D. Dedrick), UTRC, USA (D. Mosher) and FZK, Germany (M. Fichthner, participation in Task 22 will be clarified very soon). This project has also applied to IPHE.
- (2) Joint project between Univ. of Milan (A. Albinati) and Univ. of Rome (R. Cantelli) in Italy.
- (3) Joint project between UBIQEN/AIST, Japan (N. Kuriyama) and Hy-Energy, USA (K. Gross)
- (4) Proposed as a joint project between EMPA, Switzerland (A. Züttel) and FZK, Germany (M. Fichthner, participation in Task 22 will be clarified very soon).